Exact Polynomial Eigensolutions of the Schrödinger Equation for the Pseudoharmonic Potential

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Abstract

The polynomial solution of the Schrödinger equation for the Pseudoharmonic potential is found for any arbitrary angular momentum l. The exact bound-state energy eigenvalues and the corresponding eigen functions are analytically calculated. The energy states for several diatomic molecular systems are calculated numerically for various principal and angular quantum numbers. By using a proper transformation, this problem can be also solved very simply using the known eigensolutions of anharmonic oscillator potential.

I. INTRODUCTION

The three-dimensional ($3D$) anharmonic oscillators are of great importance in different physical phenomena with many applications in molecular physics [1]. The solutions of the Schrödinger equation for any l-state for such potentials are also of much concern. Morse potential is commonly used for anharmonic oscillator. However, its wavefunction is not vanishing at the origin. On the other hand, the Mie-type and also the Pseudoharmonic potentials do vanish. The Mie-type potential has the general features of the true interaction energy [1], interatomic and inter-molecular and dynamical properties in solid-state physics [2]. The Pseudoharmonic potential may be used for the energy spectrum of linear and non-linear systems [3]. The Pseudoharmonic and Mie-type potentials [3,4] are two exactly solvable potentials other than the Coulombic and anharmonic oscillator.

The anharmonic oscillator and H-atom (Coulombic) problems have been thoroughly studied in N-dimensional space quantum mechanics for any angular momentum l. These two problems are related together and hence the resulting second-order differential equation has the normalized orthogonal polynomial function solution (cf. Ref.[5] and the references therein).

In this brief letter we will follow parallel solution to Refs.[6,7,8] and give a complete normalized polynomial solution of $3D$ Schrödinger equation with Pseudoharmonic potential, anharmonic oscillator like potential with an additional centrifugal potential barrier, for any arbitrary l-state. Further, by a proper transformation, we obtain the eigensolutions of this problem from the well-known eigensolutions of the anharmonic oscillator potential. As an application, we present some numerical results of the energy states of N_2, CO, NO and CH molecules [9].

The contents of this paper is as follows. In Section II, we give the eigensolutions of the $3D$ Schrödinger equation with Pseudoharmonic potential and calculate numerically the energy levels for various diatomic molecular systems. We also obtain the eigensolutions of the Pseudoharmonic potential from a known anharmonic eigensolutions using a proper transformation. Finally, in Section III, we give our results and conclusions.

II. SCHRÖDINGER EQUATION WITH PSEUDOHARMONIC POTENTIAL

We wish to solve the Schrödinger equation for a pseudoharmonic potential [3] given by

$$V(r) = D_0 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2, \tag{1}$$

where D_0 is the dissociation energy between two atoms in a solid and r_0 is the equilibrium intermolecular seperation.

For brevity, we write the radial part of the Schrödinger equation as

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] \psi(r, \theta, \varphi) = E_{nl} \psi(r, \theta, \varphi), \tag{2}$$

and employing the transformation $\psi(r, \theta, \varphi) = \frac{R_{nl}(r)}{r} Y_{lm}(\theta, \varphi)$, to reduce it into the form [6,7]

$$\left\{ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} + 2D_0 - \frac{D_0 r^2}{r_0^2} - \frac{D_0 r_0^2}{r^2} \right] \right\} R_{nl}(r) = 0. \tag{3}$$

Furthermore, using the dimensionless abbreviations:

$$\rho = r/r_0; \ \ \varepsilon^2 = \frac{2\mu r_0^2}{\hbar^2} (E_{nl} + 2D_0); \ \ \gamma^2 = \frac{2\mu r_0^2}{\hbar^2} D_0, \tag{4}$$

gives the following simple form equation

$$\frac{d^2 R_{nl}(\rho)}{d\rho^2} + \left[\varepsilon^2 - \gamma^2 \rho^2 - \frac{\gamma^2 + l(l+1)}{\rho^2} \right] R_{nl}(\rho) = 0. \tag{5}$$

The behaviour of the solution at $\rho = 0$, determined by the centrifugal term and its asymptotic behaviour, determined by the oscillator terms, suggests us to write:

$$R_{nl}(\rho) = \rho^q \exp(-\frac{\gamma}{2}\rho^2)g(\rho), \tag{6}$$

with the numerator of x^{-2} term equal to zero leads to

$$q = \frac{1}{2} \pm \sqrt{\left(l + \frac{1}{2} \right)^2 + \gamma^2}. \tag{7}$$

As $q > 0$, the above wavefunction vanishes at $\rho = 0$, corresponding to the strong repulsion between the two atoms. It is reasonable to set Eq.(6) into Eq.(5) and then to use, instead of ρ, the variable:

$$s = \gamma \rho^2, \tag{8}$$

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giving the general type of Kummer's (Confluent Hypergeometric) differential equation

$$sg''(s) + \left[1 + \sqrt{\left(l + \frac{1}{2}\right)^2 + \gamma^2} - s\right]g'(s)$$

$$- \frac{1}{2}\left(1 + \sqrt{\left(l + \frac{1}{2}\right)^2 + \gamma^2} - \frac{\varepsilon^2}{2\gamma}\right)g(s) = 0, \tag{9}$$

with the Kummer's function solution:

$$g(\rho) = C_{11}F_1\left(\frac{1}{2}\left(1 + \sqrt{\left(l + \frac{1}{2}\right)^2 + \gamma^2} - \frac{\varepsilon^2}{2\gamma}\right), 1 + \sqrt{\left(l + \frac{1}{2}\right)^2 + \gamma^2}; \gamma\rho^2\right)$$

$$+ C_{21}F_1\left(\frac{1}{2}\left(1 - \sqrt{\left(l + \frac{1}{2}\right)^2 + \gamma^2} - \frac{\varepsilon^2}{2\gamma}\right), 1 - \sqrt{\left(l + \frac{1}{2}\right)^2 + \gamma^2}; \gamma\rho^2\right)\rho^{-2\sqrt{\left(l+\frac{1}{2}\right)^2+\gamma^2}}. \tag{10}$$

At $\rho = 0$, the second part of the solution so that $C_2 = 0$. This clearly differs from the linear oscillator where no boundary condition exists at origin. A confluent series behaves asymptotically at large positive values of its argument as

$$_1F_1(a, c; z) \rightarrow \frac{\Gamma(c)}{\Gamma(a)}\exp(z)z^{a-c}, \tag{11}$$

leads us to write

$$R_{nl}(\rho) \rightarrow \rho^{\frac{1}{2}\pm\sqrt{\left(l+\frac{1}{2}\right)^2+\gamma^2}}\exp(-\frac{\gamma}{2}\rho^2)\exp(\gamma\rho^2)\rho^{-\left(1+\sqrt{\left(l+\frac{1}{2}\right)^2+\gamma^2}+\frac{\varepsilon^2}{2\gamma}\right)}, \tag{12}$$

which is exponentially divergent wavefunction. This divergence can be avoided, in cutting off the series in Eq.(10), by putting the parameter $a = -n$, with $n = 0, 1, 2, ...$, thus transforming the series into a polynomial of degree n. Hence

$$\frac{1}{2}\left(1 + \sqrt{\left(l + \frac{1}{2}\right)^2 + \gamma^2} - \frac{\varepsilon^2}{2\gamma}\right) = -n, \tag{13}$$

with

$$\frac{\varepsilon^2}{2\gamma} = \frac{r_0}{\hbar}\sqrt{\frac{\mu}{2D_0}}\left(E_{nl} + 2D_0\right). \tag{14}$$

Thus, solving Eqs.(13) and (14) for the energy eigenvalues gives

$$E_{nl} = -2D_0 + \frac{\hbar}{r_0}\sqrt{\frac{2D_0}{\mu}}\left[2n + 1 + \sqrt{\frac{2\mu D_0 r_0^2}{\hbar^2} + \left(l + \frac{1}{2}\right)^2}\right], \tag{15}$$

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and further from Eqs.(6), (10) and (13), we write the final form of the wavefunction as

$$\psi(r,\theta,\varphi) = N_{nl} r^{-\frac{1}{2}+\sqrt{\frac{2\mu D_0 r_0^2}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \exp\left(-\sqrt{\frac{\mu D_0}{2\hbar^2}}\frac{r^2}{r_0}\right) \times$$

$${}_1F_1\left(-n, 1+\sqrt{\frac{2\mu D_0 r_0^2}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}; \sqrt{\frac{2\mu D_0}{\hbar^2}}\frac{r^2}{r_0}\right) Y_{lm}(\theta,\varphi), \tag{16}$$

where N_{nl} is a normalization constant to be determined from the normalization condition and $Y_{lm}(\theta,\varphi) = \sin^m\theta P_n^{(m,m)}(\cos\theta)\exp(\pm im\varphi)$ is the angular part of the wave function.

On the other hand, for the sake of simplicity, we can immediately obtain the energy eigenvalues and the corresponding wave functions of the Pseudoharmonic potential by transforming Eq.(3) to another Schrödinger-like equation with $L(L+1) = l(l+1) + \frac{2\mu D_0 r_0^2}{\hbar^2}$,

$$\left[\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + \frac{2\mu}{\hbar^2}\left(E'_{nL} - B^2 r^2\right)\right] R_{nL}(r) = 0, \tag{17}$$

where

$$E'_{nL} = E_{nl} + 2D_0, \; B^2 = \frac{D_0}{r_0^2}, \; \text{and } L = \frac{1}{2}\left[-1 + \sqrt{(2l+1)^2 + \frac{8\mu D_0 r_0^2}{\hbar^2}}\right]. \tag{18}$$

At this point, we should report that Eq. (17) corresponds to the Schrödinger equation of anharmonic oscillator potential, $V(r) = B^2 r^2$, with energy levels

$$E'_{nL} = \sqrt{\frac{\hbar^2}{2\mu}}B(4n + 2L + 3), \; n = 0, 1, 2, \cdots, \tag{19}$$

and wave functions

$$\psi(r,\theta,\varphi) = A_{nL} r^L \exp\left(-\sqrt{\frac{\mu}{2\hbar^2}}Br^2\right) L_n^{(L+\frac{1}{2})}\left(\sqrt{\frac{2\mu}{\hbar^2}}Br^2\right) \sin^m\theta P_n^{(m,m)}(\cos\theta)\exp(\pm im\varphi), \tag{20}$$

where $m = -(n + L + 1)$.

Finally, in the light of transformation (18), the eigenvalues (15) and the eigen functions (16) can be easily determined from the traditional formulas (19) and (20), respectively, with the Laguerre function being expressed in terms of Kummer's function, that is, $L_n^{(\nu)}(z) = {}_1F_1(-n, \nu+1; z)$..

III. RESULTS AND CONCLUSIONS

In this work we have studied the analytical solution for a Pseudoharmonic potential. Considering this potential, the problem is reduced to a harmonic oscillator potential plus an additional centrifugal potential barrier of order $1/r^2$. The exact eigensolutions for this particular case have been obtained, in a similar way as the Hydrogenic solutions [5,8]. We have calculated the energy eigenvalues and the corresponding wave functions considering bound-states for any quantum-mechanical system of any angular momentum l bound by a pseudoharmonic potential. The present results for the potential parameters $\gamma = 0$ reduces to a Harmonic oscillator solution.

Finally, we calculate the binding energies of the Pseudoharmonic potential for N_2, CO, NO and CH diatomic molecules by means of Eq.(15) with the potential parameter values [9,10].given in Table 1. The explicit values of the energy for different values of n and l are shown in Table 2.

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TABLE I: Reduced masses and spectroscopically determined properties of N_2, CO, NO and CH diatomic molecules in the ground electronic state.

Parameters[a]	N_2	CO	NO	CH
D_0 (cm^{-1})	96288.03528	87471.42567	64877.06229	31838.08149
r_0 $(A°)$	1.0940	1.1282	1.1508	1.1198
μ (amu)	7.00335	6.860586	7.468441	0.929931

[a]The parameter values here are taken from [10].

TABLE II: Calculated energy eigenvalues of the pseudoharmonic potential for N_2, CO, NO and CH diatomic molecules with different values of n and l in eV.

State (n)	l	N_2	CO	NO	CH
0	0	0.1091559	0.1019306	0.0824883	0.1686344
1	0	0.3273430	0.3056722	0.2473592	0.5050072
	1	0.3278417	0.3061508	0.2477817	0.5085903
2	0	0.5455302	0.5094137	0.4122301	0.841380
	1	0.5460288	0.5098923	0.4126526	0.8449631
	2	0.5470260	0.5108495	0.4134977	0.8521246
4	0	0.9819045	0.9168969	0.7419718	1.5141255
	1	0.9824031	0.9173755	0.7423944	1.5177087
	2	0.9834003	0.9183327	0.7432395	1.5248701
	3	0.9848961	0.9197684	0.7445070	1.5356002
	4	0.9868903	0.9216825	0.7461969	1.5498843
5	0	1.2000916	1.1206384	0.9068427	1.8504983
	1	1.2005902	1.1211170	0.9072653	1.8540815
	2	1.2015875	1.1220742	0.9081104	1.8612429
	3	1.2030832	1.1235099	0.9093779	1.8719729
	4	1.2050774	1.1254240	0.9110678	1.8862571
	5	1.2075699	1.1278165	0.9131799	1.9040761